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The dynamic T^2 chart for monitoring feedback-controlled processes

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As manufacturing quality has become a decisive factor in global market competition, statistical quality techniques such as Statistical Process Control (SPC) are widely used in industry. With advances in information, sensing, and data collection technology, large volumes of data are routinely available in processes employing Automatic Process Control (APC) and Engineering Process Control (EPC). Although there is a growing need for SPC monitoring in these feedback-controlled environments, an effective implementation scheme is still lacking. This research provides a monitoring method, termed the dynamic T^2 chart that improves the detection of assignable causes in feedback-controlled processes.

1. Introduction

Many manufacturing processes are equipped with Automatic Process Control (APC) and Engineering Process Control (EPC) capabilities, such as feedback control, to reduce short-term variation. However, for long-term process improvement, Statistical Process Control (SPC) techniques are still needed to detect any out-of-control conditions and remove their root causes. In the past, SPC and APC have been developed in parallel with little interaction between researchers in the two areas. Although the concept of combining SPC and APC was suggested decades ago, this issue has received very little attention until recently (Box and Kramer, 1992; Montgomery *et al*., 1994; Tsung and Shi, 1999). How SPC and APC can be integrated to take advantage of both of their strengths is now an important subject for both academics and practitioners (Woodall and Montgomery, 1999).

SPC monitoring of a feedback-controlled process (also called a close-loop process) is usually not effective, because feedback control action causes the output of the process to adapt to process changes. An alternative to monitoring the feedback-controlled process is to apply SPC techniques to the control action of the controlled process as suggested in Faltin and Tucker (1991) and Messina *et al*. (1996). As the control action compensates for process changes, monitoring the control action may more effectively detect these changes. Moreover, Tsung *et al*. (1999) showed that joint monitoring of both the process output and control action using bivariate charts such as Hotelling's approach may outperform many conventional SPC approaches. However, its sensitivity to process change can be further improved by considering the effects of dynamics and autocorrelation due to feedback adjustment.

In this research, we propose to improve the detectability of joint monitoring schemes using dynamic T^2 statistics that take into consideration the effects of dynamics and autocorrelation due to feedback control. In Section 2, we discuss some technical challenges in process monitoring due to feedback control. In Section 3, the dynamic T^2 monitoring scheme is proposed. Guidelines for determining the time shift factor and the covariance matrix, which are critical in designing and implementing the proposed scheme, are provided in Sections 4 and 5. In Sections 6 and 7, we analyze the performance of dynamic T^2 monitoring for mean-shift detection, and for model-change detection. Section 8 concludes the paper with some recommendations.

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2. Challenges of SPC due to feedback control

Some technical challenges need to be addressed in order to develop effective SPC methods for a feedback-controlled process.

One challenge is the existence of the "Window of Opportunity" (WO) for detection. Wardell *et al.* (1994) indicate that the application of Shewhart control charts to forecast errors in an autocorrelated process may result in poor detection of process changes, as there is only a limited period during which the process changes can be detected. SPC for open-loop autocorrelated processes and SPC for closed-loop processes both suffer from the WO problem. However, the nature and cause of the WO are different. For open-loop autocorrelated processes, the WO is due to the forecast recovery phenomenon (Superville and Adams, 1994; Apley and Shi, 1998) that occurs when there is high positive autocorrelation and residual-based control charts are used. Closed-loop processes may also suffer from the same WO problem, as feedback-controlled processes are usually autocorrelated. In addition, they suffer from a second WO problem due to the fact that mean shifts are compensated by the feedback control action and there is only a short window for detection (Box and Kramer, 1992). All conventional SPC techniques suffer from these problems. In this paper, we focus on the second WO problem. Tsung *et al.* (1999) indicated that this problem may be alleviated by monitoring the input, as well as the output. Fig. 1(a) illustrates how a feedback controller eliminates the mean-shift in the controlled output. The control input in Fig. 1(b), however, experiences a sustained mean-shift. This is an insight as to why we are monitoring both the input and output.

Another challenge is the impact of dynamics and autocorrelation due to feedback control, which cannot be handled by most conventional SPC methods. Most conventional methods were developed for monitoring processes in their steady-state operation under an assumption of time independence. Consequently, lack of autocorrelation and stationarity must be established before utilizing these methods. However, the statistical basis for these methods is lost in feedback-controlled processes because they are usually autocorrelated due to feedback adjustment. Hence, misleading results may be generated. In the existing literature, most studies on autocorrelated SPC focus on processes without feedback control, and usually consider how to reduce the effects of dynamics and autocorrelation (see Wardell *et al.* (1994) and references therein). Even the joint monitoring schemes proposed by Tsung *et al.* (1999) did not take advantage of the dynamic relation between input and output. Here we extend the joint monitoring scheme by monitoring a dynamic T^2 that incorporates information on the process dynamics and autocorrelation.

3. Methodology

Consider the process under feedback control shown in Fig. 2, and assume without loss of generality that the target value is zero. The measured output y_t can be

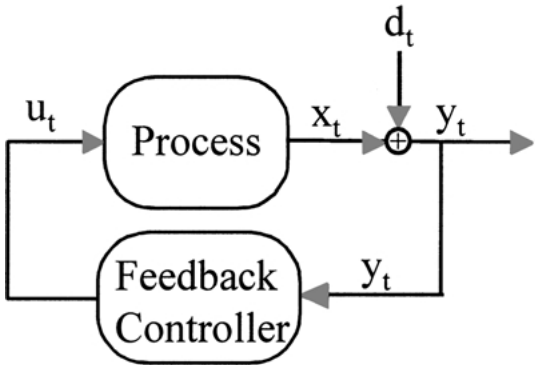

Fig. 2. Block diagram of a feedback-controlled process.

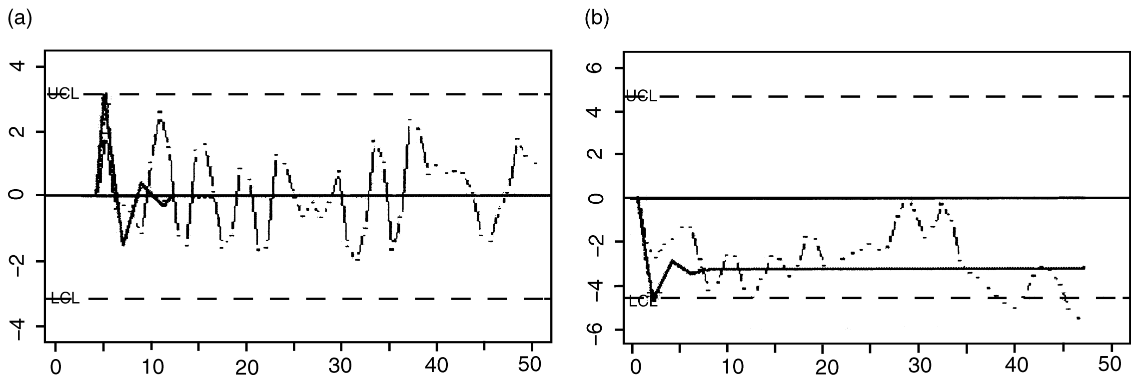

Fig. 1. Shewhart charts for: (a) the feedback-controlled outputs; and (b) the control actions of a ARMA(1,1) process (where $\phi = 0.7$ and $\theta = -0.3$) with PID control (where $k_P = 0.72$, $k_I = 0.53$, $k_D = -0.21$). The solid lines show their corresponding mean shifts.

viewed as the deviation from target. u_t represents the control action (i.e., the adjustable control input). y_t is the sum of two components: (i) a term x_t that depends on the control input; and (ii) the process disturbance d_t. Let u_t represent the control action, i.e., the process input, with the initial input assumed to be zero. We consider a simple dynamic model with $x_t = u_{t-1}$, where the output at run t, x_t, only depends on the input at the start of run t (end of run $t-1$), u_{t-1}. This is frequently used to model Run-To-Run (RTR) manufacturing processes such as Chemical-Mechanical Polishing (CMP) processes and epitaxial growth processes (Ingolfsson and Sachs, 1993; Del Castillo and Hurwitz, 1997), where the input immediately has its full effect on the output in one run.

The output y_t can be written as

$$y_t = x_t + d_t = u_{t-1} + d_t. \tag{1}$$

We consider an autoregressive-moving average (ARMA-(1,1)) disturbance model

$$d_t = \phi d_{t-1} + a_t - \theta a_{t-1}, \tag{2}$$

where $|\phi| < 1$, $|\theta| < 1$, and a_t represents white noise. We only consider ARMA(1,1) models because actual stationary industrial process time series can often be presented by ARMA models with orders less than two (Box *et al.*, 1994). Also, when ϕ is close to one, d_t is approximately an integrated-moving-average (IMA(0,1,1)) model, which is a popular nonstationary model (Box *et al.*, 1994). We illustrate the concepts with an ARMA(1,1) disturbance, although the method applies to higher-order ARMA disturbance models as well.

In industrial practice, Proportional-Integral-Derivative (PID) feedback control schemes are the most commonly used. The PID control law can be expressed as

$$u_t = -k_P y_t - k_I \sum_{j=0}^{\infty} y_{t-j} - k_D(y_t - y_{t-1}), \tag{3}$$

where k_P, k_I, and k_D are constants. Both Exponentially-Weighted-Moving-Average (EWMA) control and Proportional-Integral (PI) control are special cases of PID schemes in which only one or two of these three modes of action are used (Tsung *et al.*, 1998). Note that, related to the WO problem, complete steady-state compensation of mean shifts only happens when the controller has Integral control action (Astrom and Wittenmark, 1990).

To address the WO problem and consider the dynamic relations between the input and output, we propose to monitor a dynamic joint-monitoring statistic. The form is similar to the usual T^2 statistics but the data vector is composed of time shifted observations of both the input and output. This utilizes the concept of appending lagged data, which has been used in system identification and modeling (Ljung, 1999). To monitor the closed-loop process, one may consider monitoring a Dynamic T^2 statistic of the form

$$DT_t^L = \mathbf{X}_t^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} \mathbf{X}_t \tag{4}$$

where $\mathbf{X}_t = [y_t, u_t, y_{t-1}, u_{t-1}, \ldots, y_{t-L}, u_{t-L}]^{\mathrm{T}}$, $\boldsymbol{\Sigma}$ is the covariance matrix of $\mathbf{X}_t$, and L is a user-specified time shift factor. This is a more general version of the joint-monitoring procedure presented in Tsung *et al.* (1999), in which L was restricted to zero. Tsung *et al.* (1999) demonstrated that jointly monitoring the input and output is more effective than just monitoring the output at dealing with the WO problem that results from the controller compensating mean shifts in the process output. As will be shown in this paper, better performance may be achieved when $L > 0$ is used. Guidelines for selecting L and calculating $\boldsymbol{\Sigma}$ will be presented in subsequent sections of this paper.

The fact that the process is closed-loop, however, presents a problem when trying to implement the Dynamic T^2 chart for $L > 0$. Specifically, the covariance matrix $\boldsymbol{\Sigma}$ may not be invertible due to multicollinearity, in which case DT_t^L cannot be calculated. This is the direct result of using feedback control. For example, the PID control law in Equation (3) can also be expressed as

$$u_t = u_{t-1} - (k_P + k_I + k_D)y_t + (k_P + 2k_D)y_{t-1} - k_D y_{t-2}, \tag{5}$$

which sets u_t equal to a linear combination of $\{u_{t-1}, y_t, y_{t-1}, y_{t-2}\}$ for all t. If PI control is used, so that $k_D = 0$, then u_t is a linear combination of $\{u_{t-1}, y_t, y_{t-1}\}$.

To illustrate, suppose $L = 1$ and $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ u_{t-1}]^{\mathrm{T}}$. If PI control is used, the linear relationship $u_t - u_{t-1} + (k_P + k_I)y_t - (k_P)y_{t-1} = 0$ holds at every timestep. Therefore, the rank of $\boldsymbol{\Sigma}$ will only be three, and $\boldsymbol{\Sigma}$ will be noninvertible. In this case, DT_t^1 cannot be calculated. On the other hand, if PID control is used, there is no linear relationship between $\{y_t, u_t, y_{t-1}, u_{t-1}\}$. $\boldsymbol{\Sigma}$ will have full rank, and DT_t^1 can be calculated.

Now suppose $L = 2$ and $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ u_{t-1}\ y_{t-2}\ u_{t-2}]^{\mathrm{T}}$. If PI control is used, the two linear relationships $u_t - u_{t-1} + (k_P + k_I)y_t - (k_P)y_{t-1} = 0$ and $u_{t-1} - u_{t-2} + (k_P + k_I)y_{t-1} - (k_P)y_{t-2} = 0$ both hold at every timestep. Therefore, the rank of $\boldsymbol{\Sigma}$ will only be four, and DT_t^2 cannot be calculated. Even if PID control is used, the linear relationship $u_t - u_{t-1} + (k_P + k_I + k_D)y_t - (k_P + 2k_D)y_{t-1} + k_D y_{t-2} = 0$ will still hold, and $\boldsymbol{\Sigma}$ will only have rank five. DT_t^2 cannot be calculated in this case either.

For any $L > 0$, it can be shown that $\boldsymbol{\Sigma}$ will have rank $L + 2$ if PI control is used and rank $L + 3$ if PID control is used. Thus, since $\boldsymbol{\Sigma}$ is a $2(L+1) \times 2(L+1)$ matrix, it is never possible to calculate DT_t^L directly when $L \geq 2$. There are two possible solutions to this problem. The first is to eliminate some of the linearly dependent elements of $\mathbf{X}_t$. For example, if $L = 2$ and PID control is used, one could redefine $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ u_{t-1}\ u_{t-2}]^{\mathrm{T}}$. $\boldsymbol{\Sigma}$ would then be of full rank five. If $L = 2$ and PI control is used, one could redefine $\mathbf{X}_t = [y_t\ u_t\ u_{t-1}\ u_{t-2}]^{\mathrm{T}}$ or $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ y_{t-2}]^{\mathrm{T}}$. In both cases, $\boldsymbol{\Sigma}$ would be of full rank four.

When L is large, however, it may be difficult to identify exactly which elements of $\mathbf{X}_t$ are linearly dependent and must be removed. A more attractive solution is to use a generalized inverse (Rao, 1973) of $\boldsymbol{\Sigma}$ when calculating DT_t^L. Let the eigenvectors of $\boldsymbol{\Sigma}$ (taken to be an orthonormal set) be denoted $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_{2(L+1)}\}$ and let the corresponding eigenvalues be denoted $\{\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \ldots, \boldsymbol{\lambda}_{2(L+1)}\}$. It is well known that $\boldsymbol{\Sigma}$ can be represented as

$$\boldsymbol{\Sigma} = \sum_{i=1}^{2(L+1)} \boldsymbol{\lambda}_i \mathbf{e}_i \mathbf{e}_i^{\mathrm{T}}. \tag{6}$$

Furthermore, if $\boldsymbol{\Sigma}$ is full rank (which occurs if and only if all eigenvalues are strictly greater than zero), then the inverse of $\boldsymbol{\Sigma}$ is given by

$$\boldsymbol{\Sigma}^{-1} = \sum_{i=1}^{2(L+1)} \frac{1}{\boldsymbol{\lambda}_i} \mathbf{e}_i \mathbf{e}_i^{\mathrm{T}}. \tag{7}$$

In light of this, a generalized inverse of $\boldsymbol{\Sigma}$, denoted $\boldsymbol{\Sigma}^-$, is (Rao, 1973)

$$\boldsymbol{\Sigma}^{-} = \sum_{\substack{i=1\\ \lambda_i \neq 0}}^{2(L+1)} \frac{1}{\boldsymbol{\lambda}_i} \mathbf{e}_i \mathbf{e}_i^{\mathrm{T}}. \tag{8}$$

In other words, $\boldsymbol{\Sigma}^-$ is identical to (7) except that the summation is over only the positive eigenvalues.

For a given L, let $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ u_{t-1} \cdots y_{t-L}\ u_{t-L}]^{\mathrm{T}}$ as earlier, and let p denote the rank of $\boldsymbol{\Sigma}$. p is also the number of nonzero eigenvalues of $\boldsymbol{\Sigma}$. As discussed above, when PI control is used, $p = L + 2$, and when PID control is used, $p = L + 3$.

Based on this, we redefine the dynamic T^2 statistic DT_t^L as

$$DT_t^L = \mathbf{X}_t^{\mathrm{T}} \boldsymbol{\Sigma}^{-} \mathbf{X}_t. \tag{9}$$

The joint decision rule is to sound an alarm when DT_t^L is outside a user-defined control limit. Because u_t is a linear combination of the y_i's, $\mathbf{X}_t$ has a multivariate normal distribution. This implies that when the process is in-control, DT_t^L follows a chi-squared distribution with p degrees-of-freedom (Rao, 1973; result 8a.2 (viii)). Thus, an appropriate control limit CL_{DT} for DT_t^L would be $\chi^2_{\alpha,p}$.

4. Guideline for selecting L

It is critical to select an appropriate time lag parameter L for the dynamic monitoring scheme. Selecting an L smaller than necessary may lead to ineffective monitoring, as the test statistic cannot fully capture the dynamic relation between the input and output. Selecting an L larger than necessary may lead to redundant computing because of the repeated dynamic structure between the input and output. Also, as will be observed from the simulation study in a later section, the effect of L is analogous to the effect of the discount factor λ in an EWMA chart or the sample size in an X-bar chart. The larger L is, the larger the "memory", and the more data are considered in the test statistic. Thus, for large L, we expect better detection of small shifts, but slower detection of large shifts.

Apley and Tsung (2001) have considered a related problem in SPC for open-loop autocorrelated processes. Their recommendations are to select an L value by fitting an AR(∞) model to y_t. The suggested L will be the lag after which the magnitude of the AR(∞) model parameters decay to negligible values (e.g., 0.1). The AR(∞) model parameters can be easily found using the methods in Pandit and Wu (1983). The AR(∞) model parameters for the process

$$y_t = \frac{1 - \theta B}{1 - \phi B} a_t, \tag{10}$$

are the coefficients in the expansion

$$\frac{1 - \phi B}{1 - \theta B} y_t = \left(1 + \phi_1 B + \phi_2 B^2 + \phi_2 B^3 + \cdots\right) y_t = a_t, \tag{11}$$

which are given by Equation (3.1.19) of Pandit and Wu (1983) with θ and ϕ reversed. That is, the equivalent AR(∞) model is

$$y_t + \sum_{j=1}^{\infty} (\theta - \phi)\theta^{j-1} y_{t-j} = a_t. \tag{12}$$

Thus, the "best" L for ensuring $\mathbf{X}_t$ contains a full "summary" of the process dynamics would be such that $\left|(\theta - \phi)\theta^{j-1}\right| < \xi$ for $j > L$. Here, ξ would be some small number. Apley and Tsung (2000) did extensive simulations for open-loop autocorrelated processes, and found the dynamic scheme effective using this guideline with $\xi = 0.1$.

As discussed before, for $L > 0$, $\boldsymbol{\Sigma}$ will typically be noninvertible when feedback control is used. Using the generalized inverse method in the previous section gives exactly the same results as eliminating some of the linearly dependent elements of $\mathbf{X}_t$. For example, suppose PI control is used. For $L = 4$, we can see that $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ y_{t-2}\ y_{t-3}\ y_{t-4}]^{\mathrm{T}}$ has the exact same T^2 statistic as $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ u_{t-1}\ y_{t-2}\ y_{t-3}\ y_{t-4}]^{\mathrm{T}}$. This follows since the additional term u_{t-1} is linearly dependent on $\{y_t, u_t, y_{t-1}, y_{t-2}\}$ through the feedback control law at time t. Thus, we gain nothing by including the extra u_{t-1} term in $\mathbf{X}_t$. Likewise, $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ y_{t-2}\ y_{t-3}\ y_{t-4}]^{\mathrm{T}}$ and $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ y_{t-2}\ u_{t-2}\ y_{t-3}\ y_{t-4}]^{\mathrm{T}}$ have the exact same T^2 statistic, so it is not necessary to include the additional u_{t-2} term in $\mathbf{X}_t$. However, $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ y_{t-2}\ y_{t-3}\ y_{t-4}]^{\mathrm{T}}$ and $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ y_{t-2}\ y_{t-3}\ y_{t-4}\ u_{t-4}]^{\mathrm{T}}$ do not have the exact same T^2 statistic, because u_{t-4} is not linearly dependent on the other elements of $\mathbf{X}_t$. So we may gain something by including the additional u_{t-4} term. An advantage of using the generalized inverse method is that it automatically determines which additional terms in $\mathbf{X}_t$ are not linearly dependent and add information.

If one does not wish to deal with generalized inverses and large data vectors in practice, we suggest a simplified method of including only one input term in the data vector, i.e., $\mathbf{X}_t = [y_t\ u_t\ y_{t-1}\ y_{t-2} \cdots y_{t-L}]^{\mathrm{T}}$. The L value can be selected by fitting an AR(∞) model to y_t as discussed. If the feedback controller has Integral (I) control action, $\boldsymbol{\Sigma}$ will always be of full rank, and we can then use the standard T^2 statistic. Some information may be lost, however, depending on the process model and feedback control scheme.

5. Guideline for determining the covariance matrix

It is also necessary to determine the covariance matrix $\boldsymbol{\Sigma}$ for dynamic monitoring. In general, $\boldsymbol{\Sigma}$ will depend on the feedback control law that is used. One possibility is to estimate the covariance matrix from closed-loop data. We suggest, however, an alternative method that uses open-loop data as follows: (i) use open-loop data to estimate the ARMA disturbance model; (ii) determine the feedback control rule (i.e., determine k_{P}, k_{I}, and k_{D} for the PID scheme) based on the ARMA model; then (iii) calculate the covariance matrix $\boldsymbol{\Sigma}$ based on the ARMA model and feedback control rule.

A systematic procedure for calculating the covariance matrix $\boldsymbol{\Sigma}$ from the ARMA model and the PID control scheme is as follows:

From Equations (1)–(3), we have

$$y_t = (1-(1+\theta)B + \theta B^2) \times \varphi^{-1}(B) \times a_t, \tag{13}$$

and

$$\begin{aligned} u_t = {} & [(-k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}}) + (2k_{\mathrm{D}} + k_{\mathrm{P}} + \theta \times (k_{\mathrm{P}} + k_{\mathrm{I}} + k_{\mathrm{D}})) \\ & \times\ B - (k_{\mathrm{D}} + \theta \times (2k_{\mathrm{D}} + k_{\mathrm{P}}))B^2 + k_{\mathrm{D}} \times \theta B^3] \\ & \times \varphi^{-1}(B) \times a_t, \end{aligned} \tag{14}$$

where B is the backward shift operator, and

$$\begin{aligned} \varphi(B) = {} & 1 - (1 - k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}} + \phi)B \\ & - (k_{\mathrm{P}} + 2k_{\mathrm{D}} - \phi \times (1 - k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}}))B^2 \\ & - (-k_{\mathrm{D}} - \phi \times (k_{\mathrm{P}} + 2k_{\mathrm{D}}))B^3 - (\phi \times k_{\mathrm{D}})B^4. \end{aligned} \tag{15}$$

By following a derivation similar to one in Pandit and Wu (1983, p. 105), we can express both y_t and u_t in terms of their Green's function representations:

$$y_t = \sum_{j=0}^{\infty} G_j a_{t-j}, \tag{16}$$

with $G_j = g_1\lambda_1^j + g_2\lambda_2^j + g_3\lambda_3^j + g_4\lambda_4^j$, where $\lambda_1, \lambda_2, \lambda_3$ and λ_4 are the roots of

$$\begin{aligned} \varphi(B) = {} & 1 - (1 - k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}} + \phi) \\ & \times B - (k_{\mathrm{P}} + 2k_{\mathrm{D}} - \phi \times (1 - k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}})) \\ & \times B^2 - (-k_{\mathrm{D}} - \phi \times (k_{\mathrm{P}} + 2k_{\mathrm{D}}))B^3 - (\phi \times k_{\mathrm{D}})B^4 = 0, \end{aligned}$$

$$g_1 = \frac{\lambda_1^3 - (1+\theta)\lambda_1^2 + \theta \times \lambda_1}{(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)(\lambda_1 - \lambda_4)},$$

$$g_2 = \frac{\lambda_2^3 - (1+\theta)\lambda_2^2 + \theta \times \lambda_2}{(\lambda_2 - \lambda_1)(\lambda_2 - \lambda_3)(\lambda_2 - \lambda_4)},$$

$$g_3 = \frac{\lambda_3^3 - (1+\theta)\lambda_3^2 + \theta \times \lambda_3}{(\lambda_3 - \lambda_1)(\lambda_3 - \lambda_2)(\lambda_3 - \lambda_4)},$$

$$g_4 = \frac{\lambda_4^3 - (1+\theta)\lambda_4^2 + \theta \times \lambda_4}{(\lambda_4 - \lambda_1)(\lambda_4 - \lambda_2)(\lambda_4 - \lambda_3)}.$$

Similarly,

$$u_t = \sum_{j=0}^{\infty} H_j a_{t-j},$$

with $H_j = h_1\lambda_1^j + h_2\lambda_2^j + h_3\lambda_3^j + h_4\lambda_4^j$,
where

$$h_1 = \frac{(-k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}})\lambda_1^3 + (2k_{\mathrm{P}} + k_{\mathrm{D}} + \theta \times (k_{\mathrm{P}} + k_{\mathrm{I}} + k_{\mathrm{D}}))\lambda_1^2 - (k_{\mathrm{D}} + \theta \times (2k_{\mathrm{D}} + k_{\mathrm{P}}))\lambda_1 + k_{\mathrm{D}} \times \theta}{(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)(\lambda_1 - \lambda_4)},$$

$$h_2 = \frac{(-k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}})\lambda_2^3 + (2k_{\mathrm{P}} + k_{\mathrm{D}} + \theta \times (k_{\mathrm{P}} + k_{\mathrm{I}} + k_{\mathrm{D}}))\lambda_2^2 - (k_{\mathrm{D}} + \theta \times (2k_{\mathrm{D}} + k_{\mathrm{P}}))\lambda_2 + k_{\mathrm{D}} \times \theta}{(\lambda_2 - \lambda_1)(\lambda_2 - \lambda_3)(\lambda_2 - \lambda_4)},$$

$$h_3 = \frac{(-k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}})\lambda_3^3 + (2k_{\mathrm{P}} + k_{\mathrm{D}} + \theta \times (k_{\mathrm{P}} + k_{\mathrm{I}} + k_{\mathrm{D}}))\lambda_3^2 - (k_{\mathrm{D}} + \theta \times (2k_{\mathrm{D}} + k_{\mathrm{P}}))\lambda_3 + k_{\mathrm{D}} \times \theta}{(\lambda_3 - \lambda_1)(\lambda_3 - \lambda_2)(\lambda_3 - \lambda_4)},$$

$$h_4 = \frac{(-k_{\mathrm{P}} - k_{\mathrm{I}} - k_{\mathrm{D}})\lambda_4^3 + (2k_{\mathrm{P}} + k_{\mathrm{D}} + \theta \times (k_{\mathrm{P}} + k_{\mathrm{I}} + k_{\mathrm{D}}))\lambda_4^2 - (k_{\mathrm{D}} + \theta \times (2k_{\mathrm{D}} + k_{\mathrm{P}}))\lambda_4 + k_{\mathrm{D}} \times \theta}{(\lambda_4 - \lambda_1)(\lambda_4 - \lambda_2)(\lambda_4 - \lambda_3)},$$

A simpler alternative for calculating Green's functions for u_t and y_t is based on the interpretation of Green's function as the response of the system to a single pulse of unit magnitude at timestep zero (Astrom and Wittenmark, 1990). The "system" is described by the input and output equations

$$y_t = \phi y_{t-1} + u_{t-1} - \phi u_{t-2} + a_t - \theta a_{t-1},$$
$$u_t = u_{t-1} - (k_P + k_I + k_D)y_t + (k_P + 2k_D)y_{t-1} - k_D y_{t-2}.$$

If the sequence a_t in the above equations were a single pulse of unit magnitude at timestep zero, i.e.,

$$a_t = \delta_t = \begin{cases} 0 & \text{if } t \neq 0, \\ 1 & \text{if } t = 0, \end{cases}$$

then y_j and u_j would be exactly equal to G_j and H_j, respectively, for $j = 0, 1, 2, \ldots$ Specifically, G_j and H_j are solutions to the equations

$$G_j = \phi G_{j-1} + H_{j-1} - \phi H_{j-2} + \delta_j - \theta\delta_{j-1}$$
$$H_j = H_{j-1} - (k_P + k_I + k_D)G_j + (k_P + 2k_D)G_{j-1} - k_D G_{j-2},$$

with initial conditions $G_j = H_j = 0$ for $j < 0$. G_j and H_j can easily be obtained numerically using a computer to iterate these equations for $j = 0, 1, 2, \ldots$ By the definition of δ_j and the initial conditions, the equations can be simplified to

$$G_0 = 1$$
$$H_0 = -(k_P + k_I + k_D)G_0 = -(k_P + k_I + k_D),$$
$$G_1 = \phi G_0 + H_0 - \theta\delta_0 = \phi - (k_P + k_I + k_D) - \theta,$$
$$H_1 = H_0 - (k_P + k_I + k_D)G_1 + (k_P + 2k_D)G_0,$$

and, for $j > 1$,

$$G_j = \phi G_{j-1} + H_{j-1} - \phi H_{j-2},$$
$$H_j = H_{j-1} - (k_P + k_I + k_D)G_j + (k_P + 2k_D)G_{j-1} - k_D G_{j-2}.$$

Following either method for calculating Green's function, the auto-covariance of y_t at lag k can be computed by

$$\mathrm{cov}(y_t, y_{t-k}) = \sigma_a^2 \sum_{j=0}^{\infty} G_{j+k} G_j,$$

and the auto-covariance of u_t at lag k can be computed by

$$\mathrm{cov}(u_t, u_{t-k}) = \sigma_a^2 \sum_{j=0}^{\infty} H_{j+k} H_j.$$

Also, the covariance between y_t and u_t at different lags can be computed as

$$\mathrm{cov}(y_t, u_{t-k}) = \sigma_a^2 \sum_{j=0}^{\infty} G_{j+k} H_j,$$

and

$$\mathrm{cov}(u_t, y_{t-k}) = \sigma_a^2 \sum_{j=0}^{\infty} H_{j+k} G_j.$$

Therefore, all the items in the covariance matrix $\boldsymbol{\Sigma}$ can be obtained from the above computations. It is straightforward to calculate the Green's function coefficients, given the ARMA model and the feedback control rule. If the closed-loop system is stable, all terms in the above infinite summations will converge exponentially to zero. Thus, the summations can typically be truncated to 100 or fewer terms. A Matlab program for calculating the covariance matrix is available upon request from the first author.

Note that the Green's function method for finding the covariance could be easily extended to higher order ARMA models. The covariance matrix could also be obtained analytically (Tsung *et al.*, 1999), although the equations are quite complex. The proposed Green's function approach is conceptually more straightforward and has cleaner equations.

Generally, the open-loop method may provide better accuracy with fewer data than directly estimating the covariance matrix from closed-loop data. The only quantities that must be estimated are ϕ, θ, and σ_a^2. An additional advantage is that if the feedback control law is changed, the covariance matrix can be recalculated without collecting new data. However, what the sample size should be and how the random errors in the estimated ARMA parameters propagate in to the covariance matrix still warrant future study.

6. Performance analysis for mean-shift detection

To investigate the performance of the proposed monitoring scheme for mean-shift detection, we compare the Average Run Length (ARL) of the dynamic T^2 (DT^1 and DT^2) and the conventional $T^2(DT^0)$ charts for monitoring PI-controlled processes. We also compare the scheme with Shewhart individual charts for monitoring the process output and monitoring the control action. The ARLs were obtained via Monte Carlo simulation. For each process 10 000 replications were used to compute the ARL with a standard error of less than 1%. In order to make a fair comparison, the control limits are adjusted so that the ARL is the same for all charts when there is no shift in the mean. In this study the in-control ARL of 200 is used. The control limits varied depending on the disturbance model parameters, the feedback control parameters, and the time lag L. One could also select the Dynamic T^2 chart control limits to provide a desired α-error, as discussed in Section 3. The in-control ARL was fixed in the simulations in order to provide a basis for comparison. Mean shifts of size 0.5, 1, 1.5, 2, 2.5, and 3 standard deviations of $d_t(\sigma_d)$ were added to the PI-controlled process, and the different monitoring schemes were applied.

The combinations of ϕ and θ that have positive autocorrelations are those that would most likely be encountered in actual manufacturing environments (Wardell *et al.*, 1994), especially with positive ϕ and smaller θ. Based on that, we choose eight combinations of the ARMA parameters in order to cover a reasonable range of the parameter space. Table 1 shows that in many cases the detection performance for DT^0, DT^1 and DT^2 is much

Table 1. ARL values of different monitoring schemes for various PID-controlled ARMA(1,1) processes under mean shifts

Process	*Mean shift*	*Individual monitoring of output*	*Individual monitoring of input*	*Joint monitoring by DT^0*	*Joint monitoring by DT^1*	*Joint monitoring by DT^2*
(I)	0.5	187.80	142.90	130.76	132.17	127.96
$\phi = 0.9$, $\theta = 0.4$,	1	161.73	59.67	57.87	56.09	54.10
$k_P = 0.06$, $k_I = 0.48$	1.5	105.76	26.44	24.17	22.75	22.66
$\mathrm{corr}(y_t, u_t) = -0.31$	2	47.49	12.28	9.48	8.25	8.94
	2.5	12.66	6.13	3.70	2.84	3.76
	3	3.06	3.43	1.65	1.33	2.31
(II)	0.5	180.26	149.54	137.65	138.22	135.50
$\phi = 0.9$, $\theta = -0.4$,	1	74.23	67.97	58.40	63.36	62.57
$k_P = 0.06$, $k_I = 1.29$	1.5	7.67	27.99	19.21	23.97	25.70
$\mathrm{corr}(y_t, u_t) = -0.74$	2	1.13	9.04	4.77	6.38	8.70
	2.5	1.00	2.64	1.45	1.63	3.47
	3	1.00	1.18	1.03	1.03	2.06
(III)	0.5	196.16	99.28	141.19	124.66	113.76
$\phi = 0.7$, $\theta = 0.3$,	1	180.61	29.55	65.93	46.52	39.55
$k_p = 0.21$, $k_I = 0.21$	1.5	146.38	13.04	26.52	16.57	14.67
$\mathrm{corr}(y_t, u_t) = -0.34$	2	97.19	7.47	10.81	6.39	6.25
	2.5	48.67	4.84	4.96	2.64	3.22
	3	17.07	3.34	2.45	1.44	2.27
(IV)	0.5	189.61	148.13	114.52	109.34	105.94
$\phi = 0.7$, $\theta = -0.3$,	1	158.97	54.33	44.46	41.78	40.33
$k_P = 0.21$, $k_I = 0.85$	1.5	104.55	21.97	17.00	16.05	16.31
$\mathrm{corr}(y_t, u_t) = -0.71$	2	45.79	9.85	6.74	6.44	7.15
	2.5	12.95	4.71	2.94	2.64	3.63
	3	2.78	2.38	1.54	1.38	2.40
(V)	0.5	111.07	112.25	111.26	105.32	99.80
$\phi = 0.5$, $\theta = 0.2$,	1	41.43	42.66	42.46	34.81	31.54
$k_P = 0.27$, $k_I = 0.00$	1.5	16.06	17.57	17.47	12.30	11.05
$\mathrm{corr}(y_t, u_t) = -0.28$	2	6.60	7.95	7.91	4.78	4.76
	2.5	2.97	3.99	3.97	2.17	2.71
	3	1.61	2.23	2.22	1.33	2.15
(VI)	0.5	192.30	74.50	127.14	118.95	106.62
$\phi = 0.5$, $\theta = -0.2$,	1	168.23	24.34	52.73	41.18	35.88
$k_P = 0.50$, $k_I = 0.12$	1.5	121.85	11.61	20.70	14.62	13.20
$\mathrm{corr}(y_t, u_t) = -0.61$	2	68.19	6.46	8.75	5.67	5.80
	2.5	25.74	3.71	4.08	2.40	3.10
	3	7.07	2.26	2.08	1.37	2.26
(VII)	0.5	107.84	109.04	103.71	103.21	98.50
$\phi = 0.3$, $\theta = 0.1$,	1	38.10	39.28	37.57	31.47	28.00
$k_P = 0.19$, $k_I = 0.00$	1.5	14.40	15.72	15.12	10.62	9.42
$\mathrm{corr}(y_t, u_t) = -0.19$	2	5.83	7.05	6.84	4.07	4.06
	2.5	2.67	3.55	3.45	1.97	2.50
	3	1.51	2.08	2.04	1.27	2.10
(VIII)	0.5	116.17	117.37	114.55	109.24	104.08
$\phi = 0.3$, $\theta = -0.1$,	1	44.49	45.92	45.11	36.29	32.78
$k_P = 0.36$, $k_I = 0.00$	1.5	17.18	18.81	18.47	12.73	11.43
$\mathrm{corr}(y_t, u_t) = -0.36$	2	6.90	8.36	8.19	4.94	4.88
	2.5	3.02	4.11	4.06	2.20	2.76
	3	1.62	2.27	2.25	1.35	2.17

better than that of individual monitoring of the output or the input. When both ϕ and θ are small, the advantage of dynamic T^2 monitoring over individual monitoring is not as significant. It is even inferior for some cases. This is because the feedback control has less impact on the process with little or low autocorrelation.

Overall, the performance of dynamic T^2 monitoring using DT^1 and DT^2 is better than that of static joint monitoring by DT^0. However, for processes (II) and (IV), the advantage of dynamic T^2 monitoring over static joint monitoring is not as significant. This can be explained in part by the correlation between the process output and control action. For a process with a small to medium correlation between the output and input, the dynamic monitoring shows improved performance. For a process with a large correlation, DT^0, DT^1 and DT^2 may have similar performances.

More specifically, DT^1 is consistently better than the other schemes for large mean shifts, while DT^2 is consistently better than the other schemes for small mean shifts. This is consistent with the discussion in Section 4, which suggested that the larger L is, the larger the "memory" is. Thus, we expect a better detection of small shifts for large L, but a better detection of large shifts for small L.

Note that for processes (III) and (VI) the ARL of the Shewhart chart monitoring the input is smaller than that of the other schemes for cases when the shift is small. Some discussion on the superiority of monitoring the input in certain cases can be found in Tsung *et al.* (1999).

7. Model-change detection and controller retuning

If the disturbance model changes, controller effectiveness may seriously degrade. Therefore, it is desirable to detect changes in the model parameters, so that the controller may be retuned appropriately. We expect that the dynamic T^2 statistic will also be sensitive to changes in parameters of the ARMA model for the disturbance process. This follows since the covariance matrix of $\mathbf{X}_t$ will depend on the ARMA model parameters. Thus, if the model changes, the covariance matrix will change from what was estimated in the past, and the T^2 statistic may sound an alarm. In this case, the users would want to "retune" their feedback controller to achieve optimum performance. For example, when there is a change in the ARMA parameters from ($\phi = 0.5$, $\theta = 0.2$) to ($\phi = 0.9$, $\theta = 0.3$), the PI control performance (with $k_P = 0.27$ and $k_I = 0.00$) substantially worsens with the process output mean squared error almost doubling from 1.02 to 1.99.

The simulation results in Table 2 show the sensitivity of the dynamic T^2 statistic to disturbance model changes, where $\Delta\phi$ is the size of a positive change in the disturbance parameter ϕ. For most of the cases the performance of dynamic T^2 monitoring by DT^1 and DT^2 is

Table 2. ARL values of different monitoring schemes for various PID-controlled ARMA(1,1) processes experiencing a disturbance model change

	$\Delta\phi$	*Individual monitoring of output*	*Joint monitoring by DT^0*	*Joint monitoring by DT^1*	*Joint monitoring by DT^2*
$\phi = 0.7$, $\theta = 0.3$,	0.1	177.14	134.37	114.71	103.57
$k_P = 0.21$, $k_I = 0.21$	0.15	156.91	96.30	76.71	68.47
	0.2	131.36	62.67	49.90	44.46
	0.25	106.44	40.40	32.88	30.17
$\phi = 0.7$, $\theta = -0.3$,	0.1	212.13	84.48	77.28	73.80
$k_P = 0.21$, $k_I = 0.85$	0.15	214.93	54.88	50.67	48.40
	0.2	217.60	37.45	34.35	32.98
	0.25	217.60	25.56	23.84	23.26
$\phi = 0.5$, $\theta = 0.2$,	0.1	163.54	163.06	154.51	147.62
$k_P = 0.27$, $k_I = 0.00$	0.15	141.20	140.57	123.78	114.61
	0.2	115.09	114.83	93.41	84.44
	0.25	88.58	88.28	68.90	61.41
$\phi = 0.5$, $\theta = -0.2$,	0.1	158.46	140.61	128.90	115.85
$k_P = 0.50$, $k_I = 0.12$	0.15	134.28	114.67	95.82	84.24
	0.2	111.09	88.68	70.47	62.21
	0.25	89.30	66.42	52.05	46.03
$\phi = 0.3$, $\theta = 0.1$,	0.1	186.17	176.37	180.13	177.64
$k_P = 0.19$, $k_I = 0.00$	0.15	171.50	161.58	156.98	150.87
	0.2	152.03	145.21	131.40	122.83
	0.25	132.61	126.42	106.65	97.49
$\phi = 0.3$, $\theta = -0.1$,	0.1	178.06	174.41	167.32	162.82
$k_P = 0.36$, $k_I = 0.00$	0.15	159.91	156.76	141.71	133.23
	0.2	141.13	138.66	116.83	107.36
	0.25	119.60	117.94	92.12	83.53

better than that of static joint monitoring by DT^0 or the individual monitoring of the output. The advantage of dynamic T^2 monitoring is more significant when the parameter change is larger. DT^2 monitoring, in particular, is consistently better than the other schemes in detecting different scales of disturbance parameter change.

Additional simulations have indicated that negative changes in ϕ and changes in θ have little impact on the controller effectiveness and that the monitoring schemes are insensitive to changes of this nature.

When the Dynamic T^2 chart sounds an alarm, it is important to know if it was caused by a mean-shift or a model-change. If it is a change in the mean, the user would want to follow-up an alarm with SPC-type corrective action. On the other hand, if the signal is caused by a change in the ARMA model parameters, the user would follow-up by retuning the controller. A simple method of diagnosis would be to use scatter plots of pairs of elements of $\mathbf{X}_t$, with the in-control $(1-\alpha)$ constant probability ellipses shown also. The $1-\alpha$ constant probability ellipse for a 2-dimensional Multivariate Normal vector with mean vector $\boldsymbol{\mu}_0$ and covariance matrix $\boldsymbol{\Sigma}_0$ is

$$\left\{x : [\mathbf{x}-\boldsymbol{\mu}_0]^{\mathrm{T}}\boldsymbol{\Sigma}_0^{-1}[\mathbf{x}-\boldsymbol{\mu}_0] = \chi^2_{\alpha,2}\right\}.$$

The following examples illustrate the idea with an ARMA(1,1) process ($\phi = 0.5$, $\theta = -0.2$) under PI control ($k_{\mathrm{P}} = 0.50$ and $k_{\mathrm{I}} = 0.12$). For $L = 0$, the in-control mean and covariance matrix of $\mathbf{X}_t$ are $\boldsymbol{\mu}_0 = [0\ 0]^{\mathrm{T}}$ and

$$\boldsymbol{\Sigma}_0 = \begin{bmatrix} 1.10 & -0.61 \\ -0.61 & 0.55 \end{bmatrix}.$$

The ellipse shown in each figure is the 95% probability ellipse when the process is in-control. Figure 3 shows 200 observations when the process mean changes from zero to $3\sigma_d$.

Figure 4 shows 200 observations when the ARMA(1,1) parameters change from ($\phi = 0.5$, $\theta = -0.2$) to ($\phi = 0.9$, $\theta = -0.3$). Although the means of the elements of $\mathbf{X}_t$ do not change, the covariance matrix of $\mathbf{X}_t$ changes to

$$\boldsymbol{\Sigma}_0 = \begin{bmatrix} 2.43 & -1.36 \\ -1.36 & 4.63 \end{bmatrix}.$$

Note that an increase in the variance of the process can also cause a change in the covariance matrix. A change in

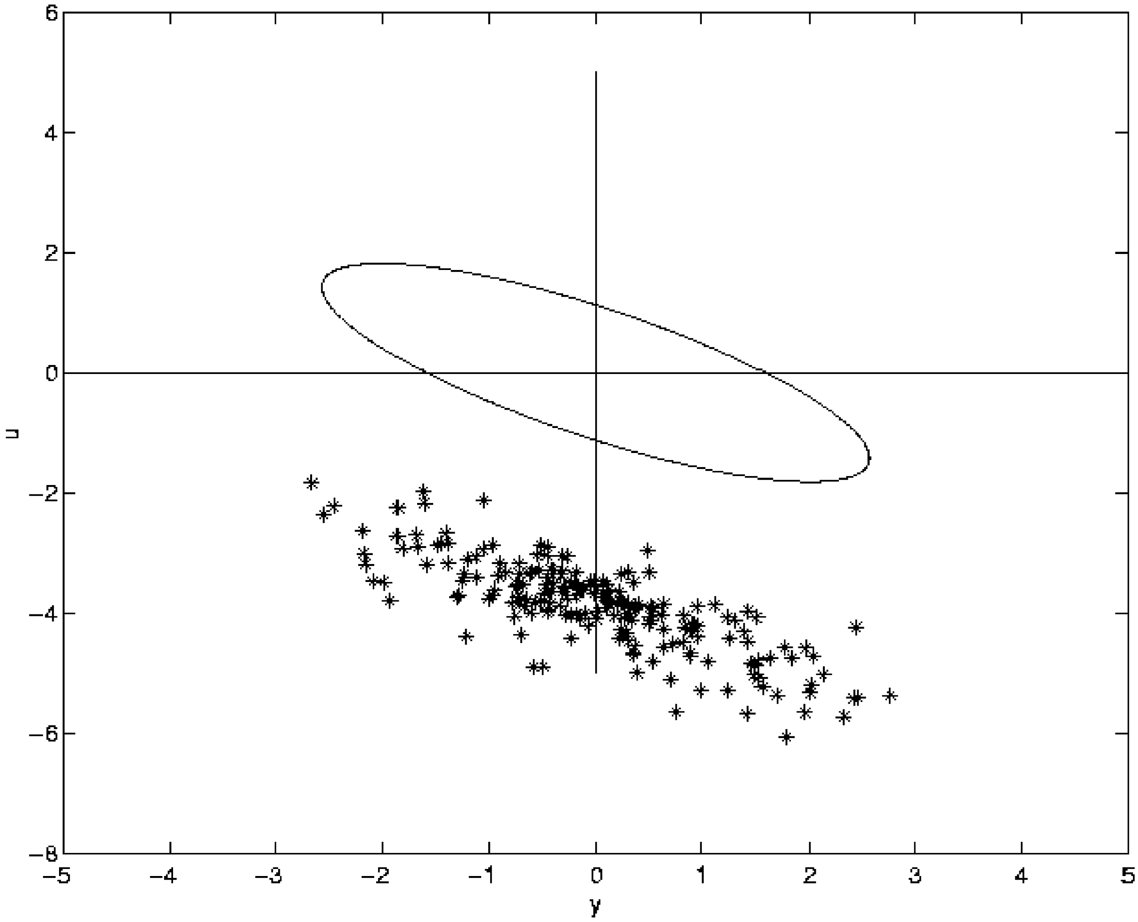

Fig. 3. A scatter plot for a feedback-controlled process when its mean changes.

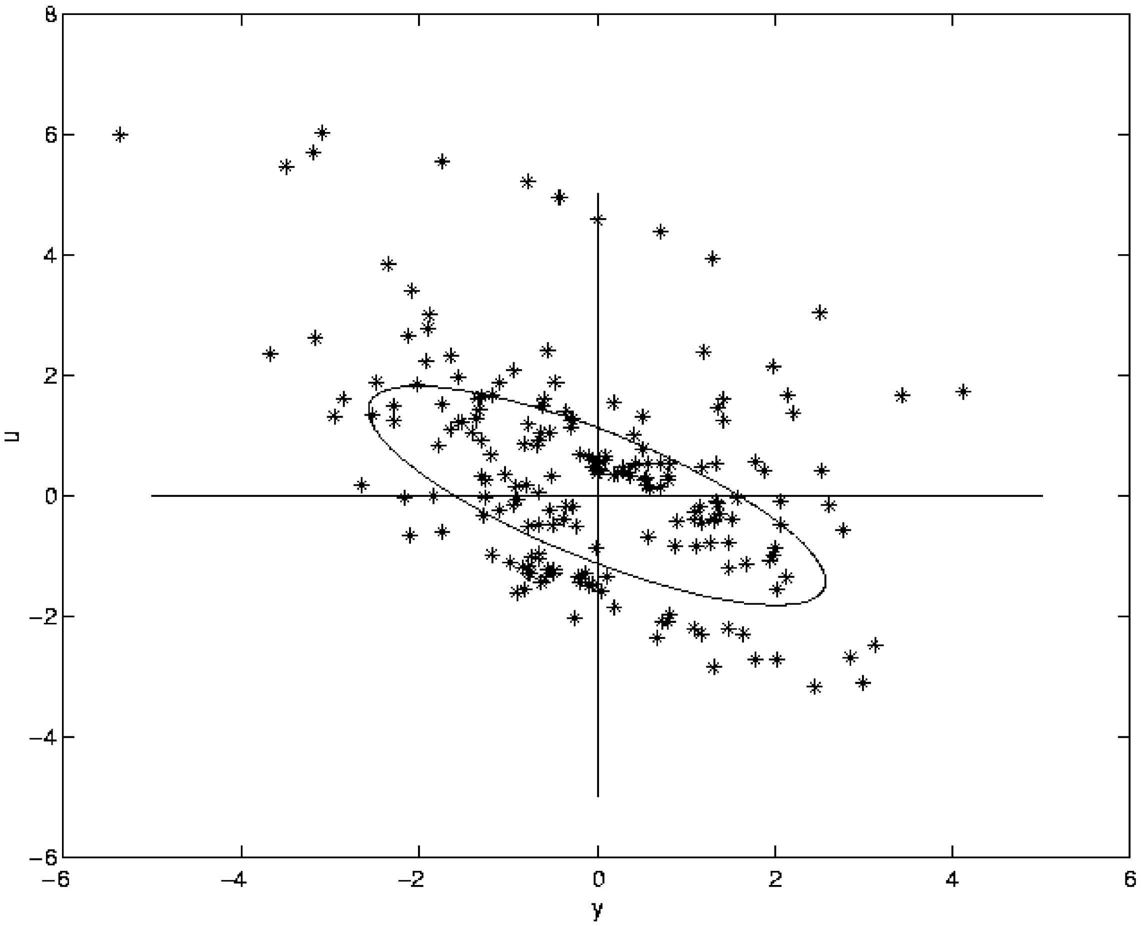

Fig. 4. A scatter plot for a feedback-controlled process when its disturbance parameter changes.

$\sigma_a{}^2$ would only affect the "scale" of the covariance matrix, while a change in the disturbance parameter would cause both a "re-scaling" and a "rotation". However, this may be difficult to distinguish in a simple scatter plot. More advanced statistical methods may be required to clarify between the similar change patterns for effective diagnosis. A retrospective diagnosis procedure was proposed by Tsung (2000).

8. Conclusion

This paper investigates process monitoring problems in an APC and SPC integrated environment. A joint monitoring scheme using dynamic T^2 statistics was proposed to improve assignable cause detectability for a feedback-controlled process. Guidelines for designing and implementing the proposed monitoring scheme are provided. The ARL performance analysis shows that the dynamic T^2 monitoring scheme is effective in detecting both mean shifts and changes in the process model parameters. How to monitor the variance of a feedback-controlled process warrants further study.

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